

Fig. 1

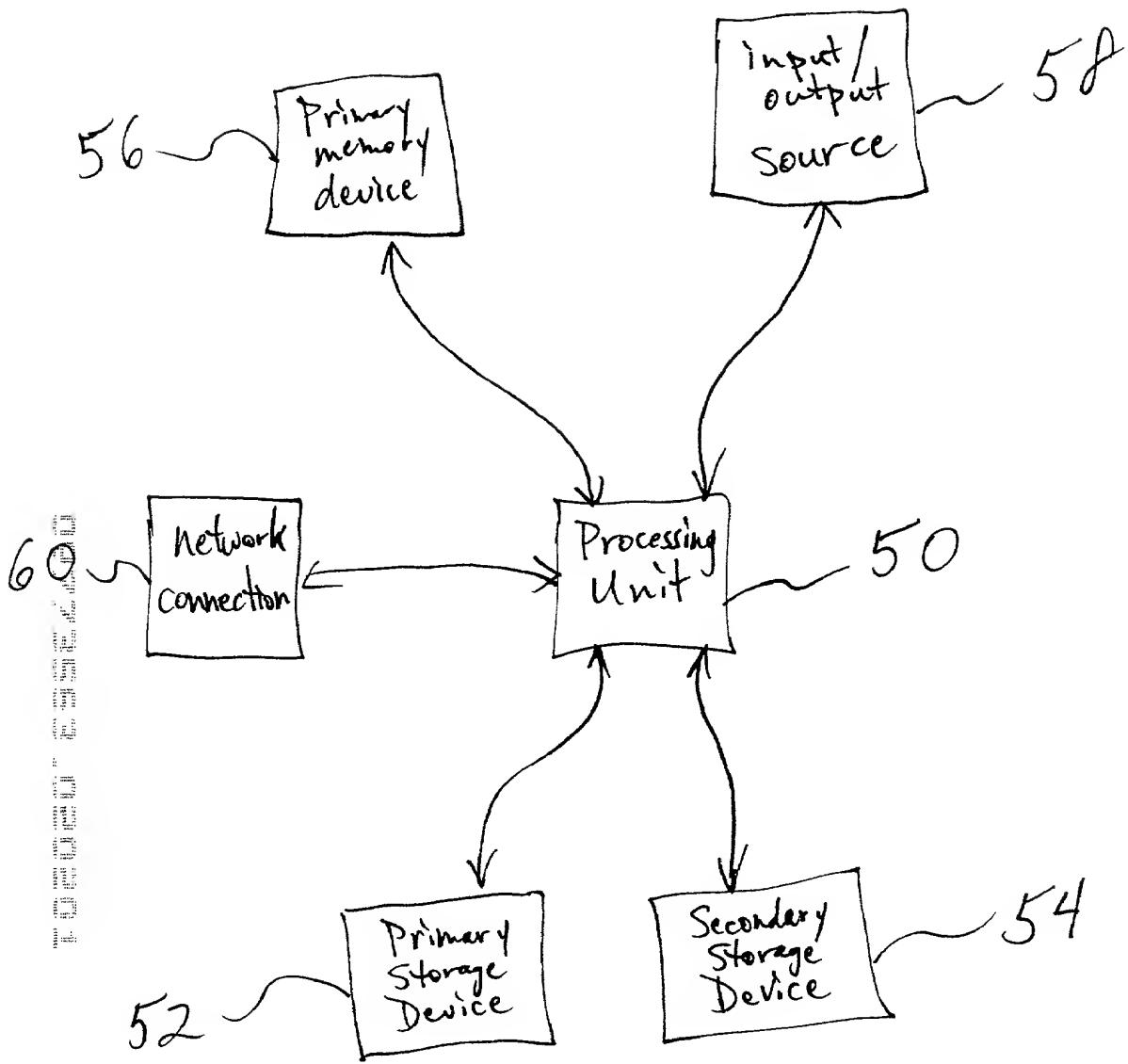


Fig. 2

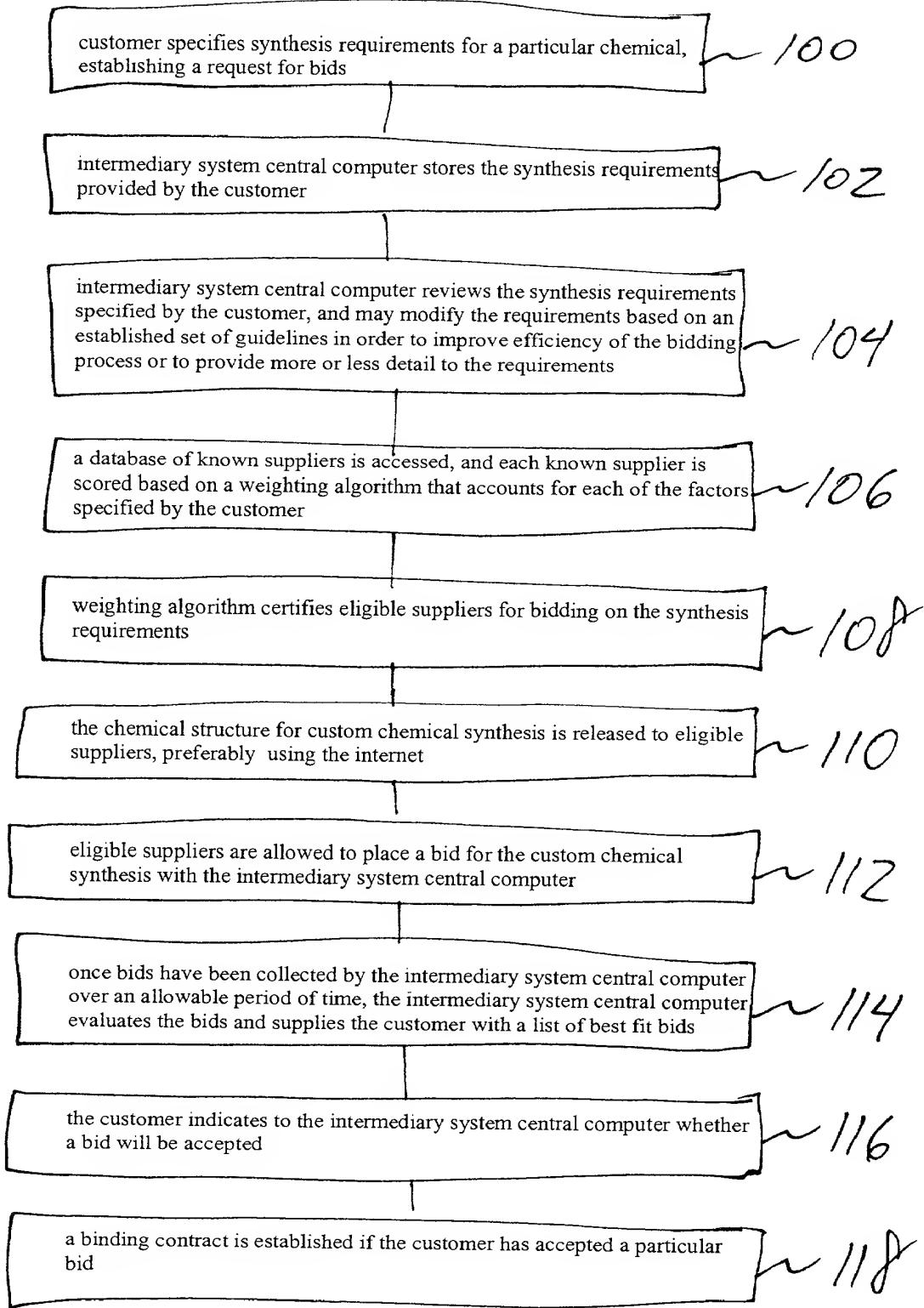


Fig. 3

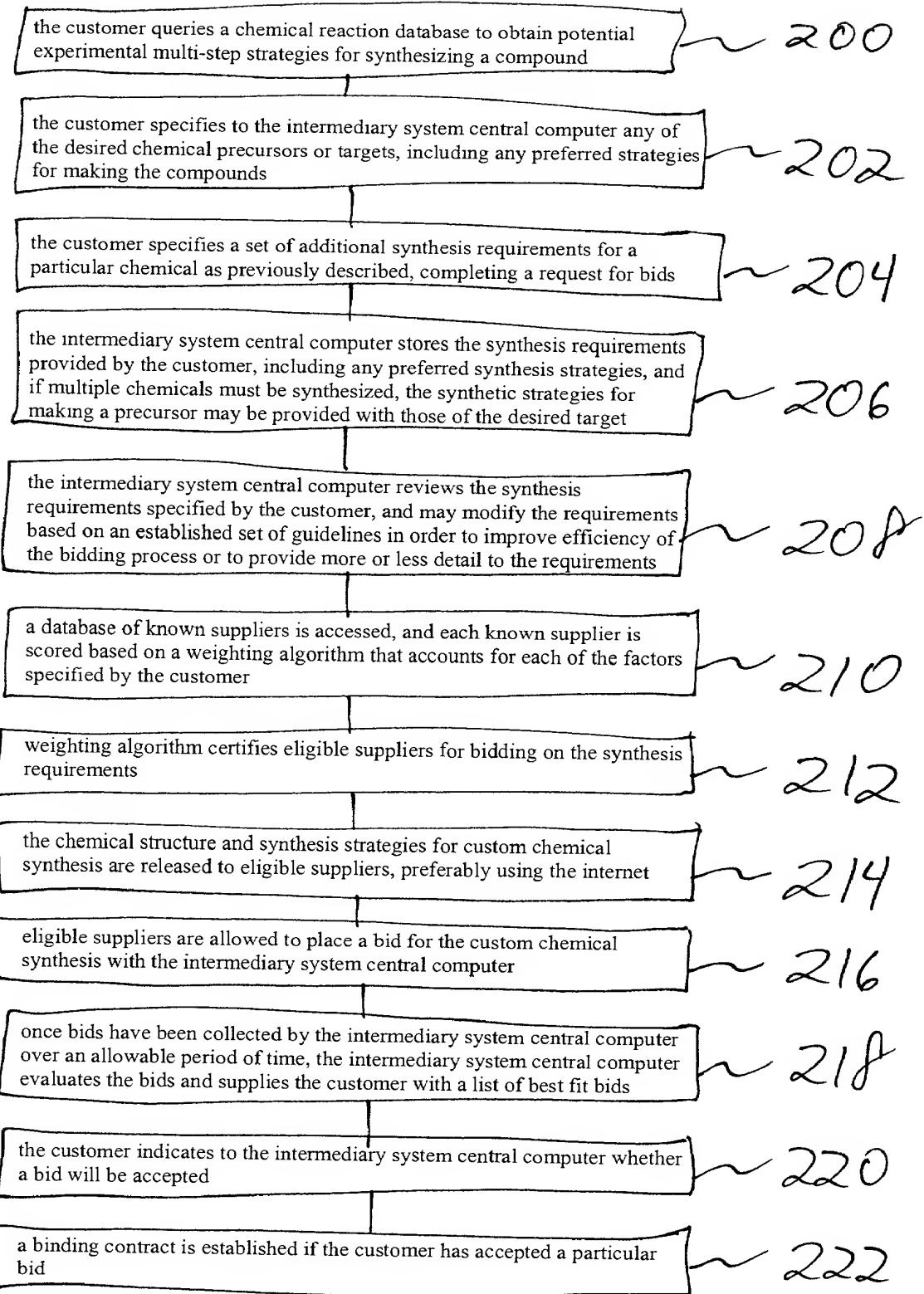


Fig. 4

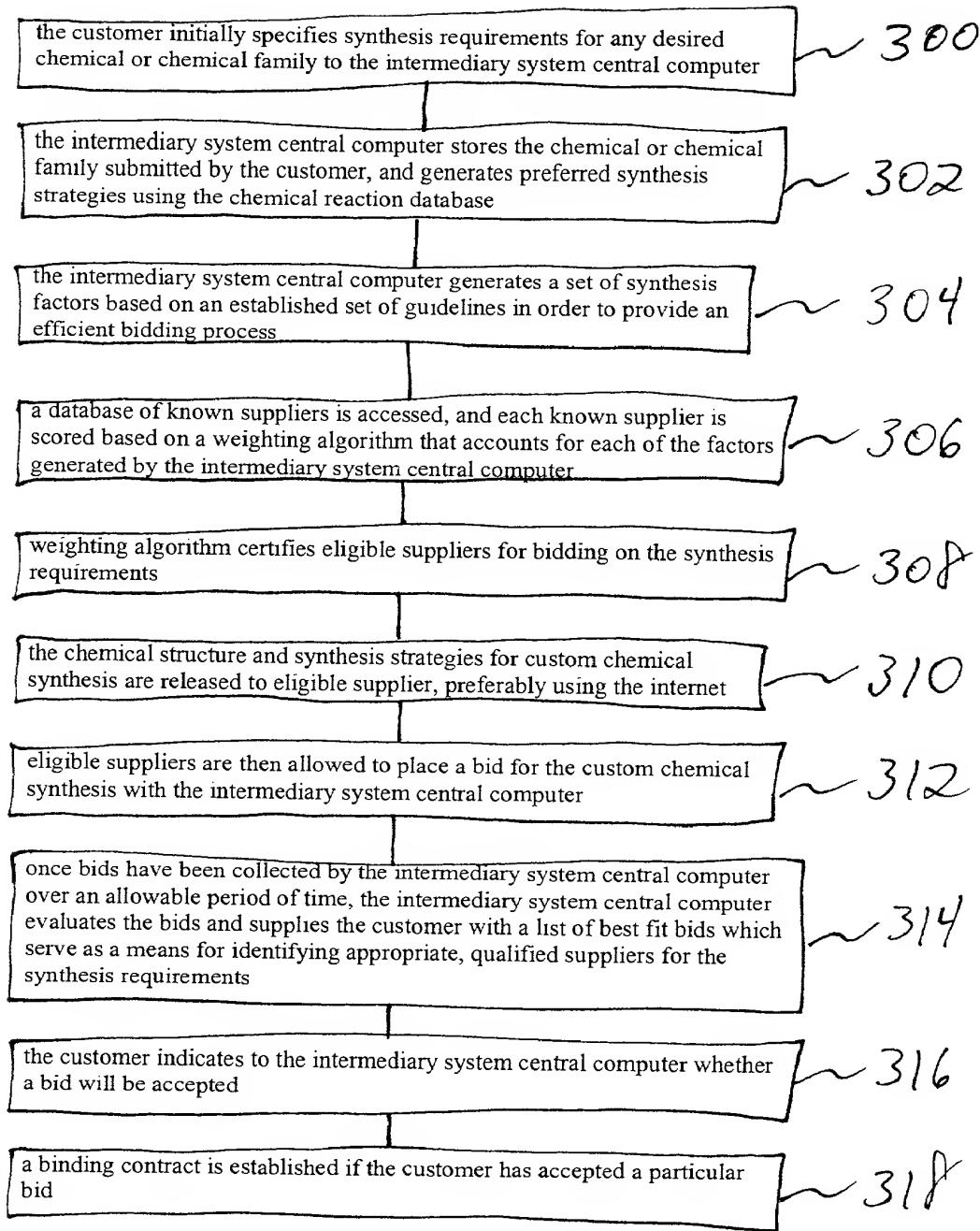


Fig. 5

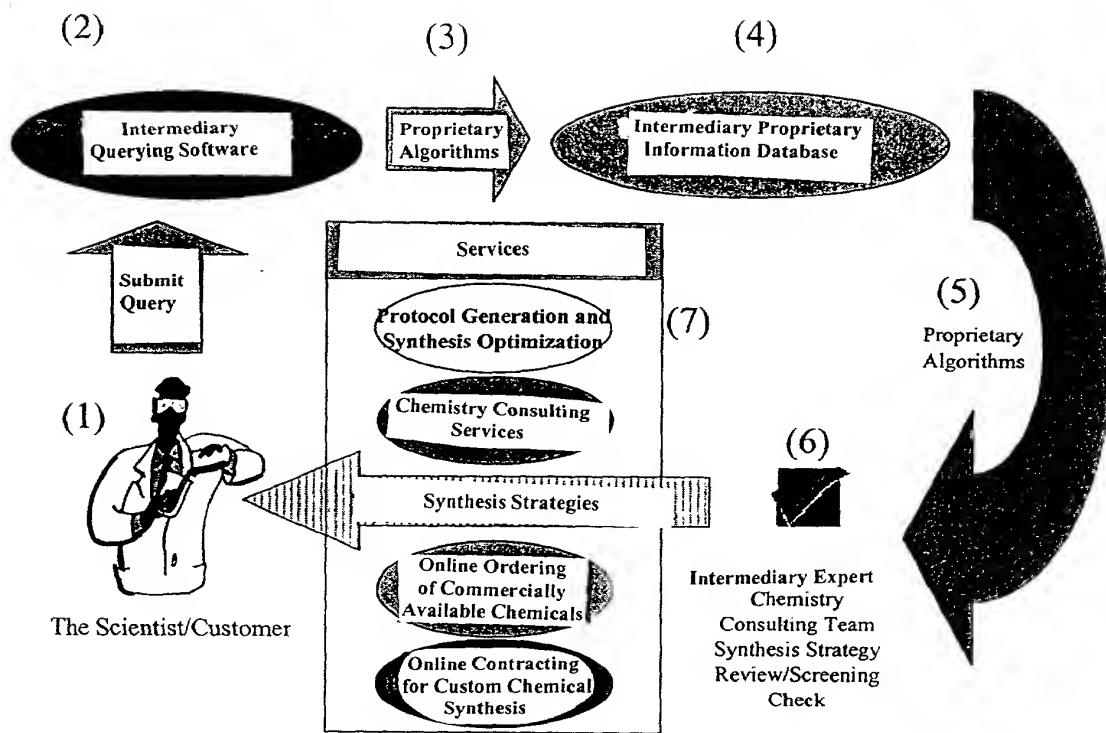
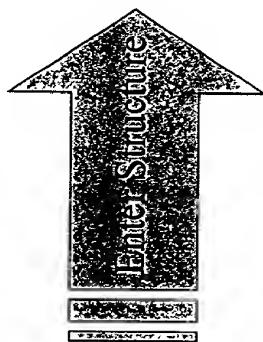
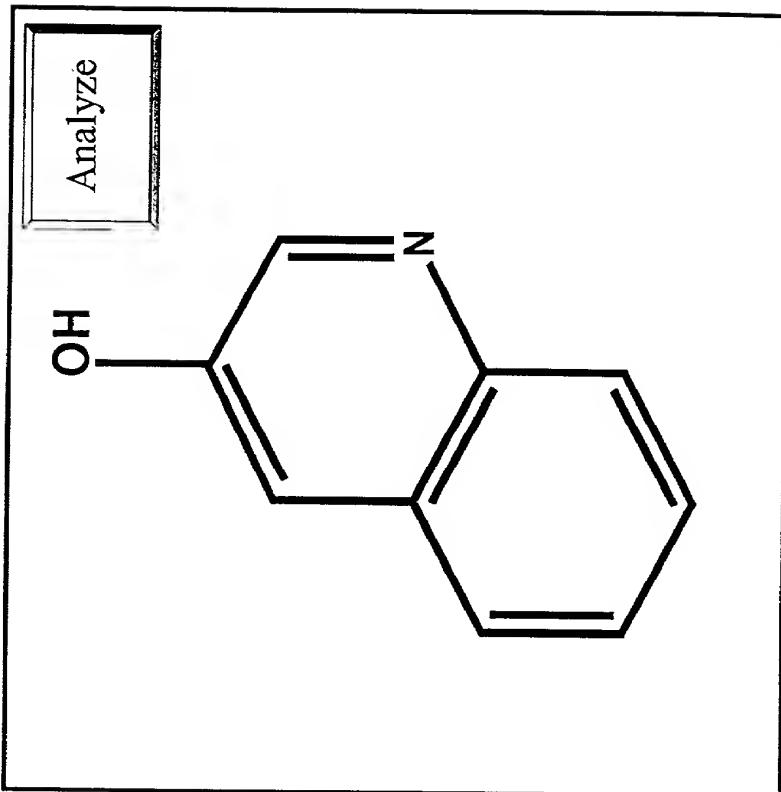


Fig. 6



Target Structure Entry



400

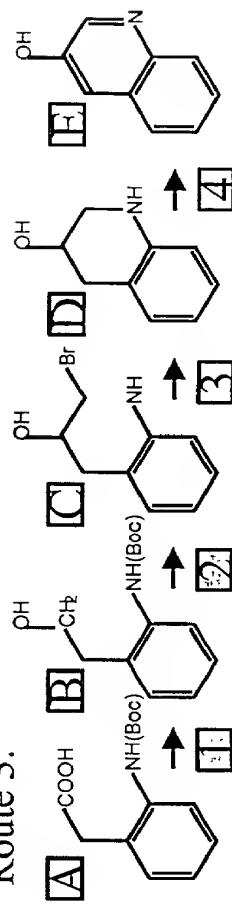
Fig. 7

Synthesis Strategies

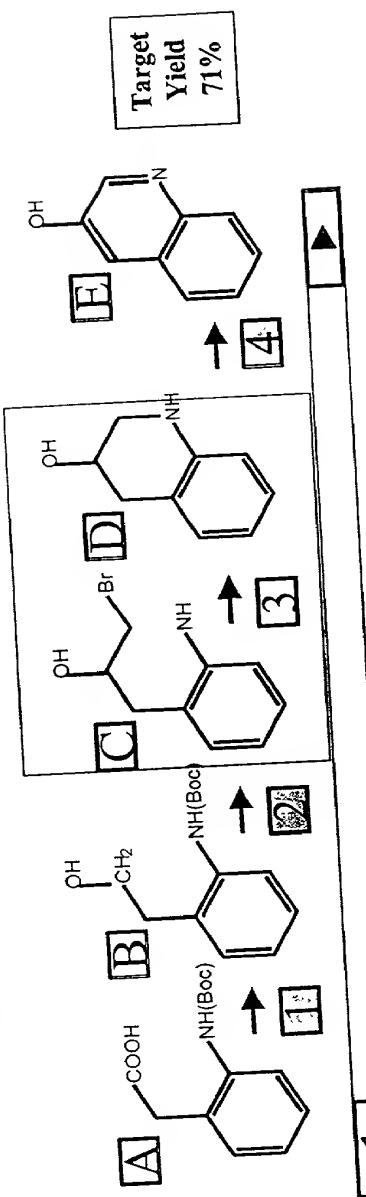
Routes	Yield %	# of steps to ACD	Purification Steps Required	Cost per mg of product	Add Synthetic Routes to Project
Route 1	86	6	4	\$2,000	☒
Route 2	75	N/A	N/A	N/A	☒
Route 3	71	4	3	\$6,434	☒
Route 4	63	5	2	\$200	☒
Route 5	44	10	8	\$22,050	☐
Route 6	31	7	6	\$15,427	☐
Route 7	24	5	5	\$155	☐
Route 8	20	6	4	\$4,450	☐
Route 9	17	6	5	\$344	☐
Route 10	9	N/A	N/A	N/A	☐
Route 11	4	6	6	\$36,000	☐

120

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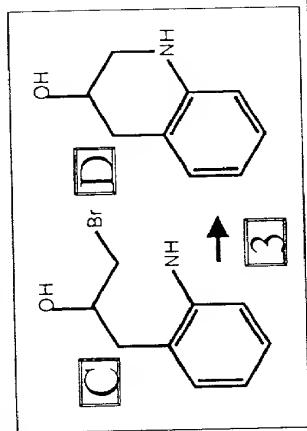
Synthesis Reaction Planner



440

Fig. 9

Synthesis Protocol Generation



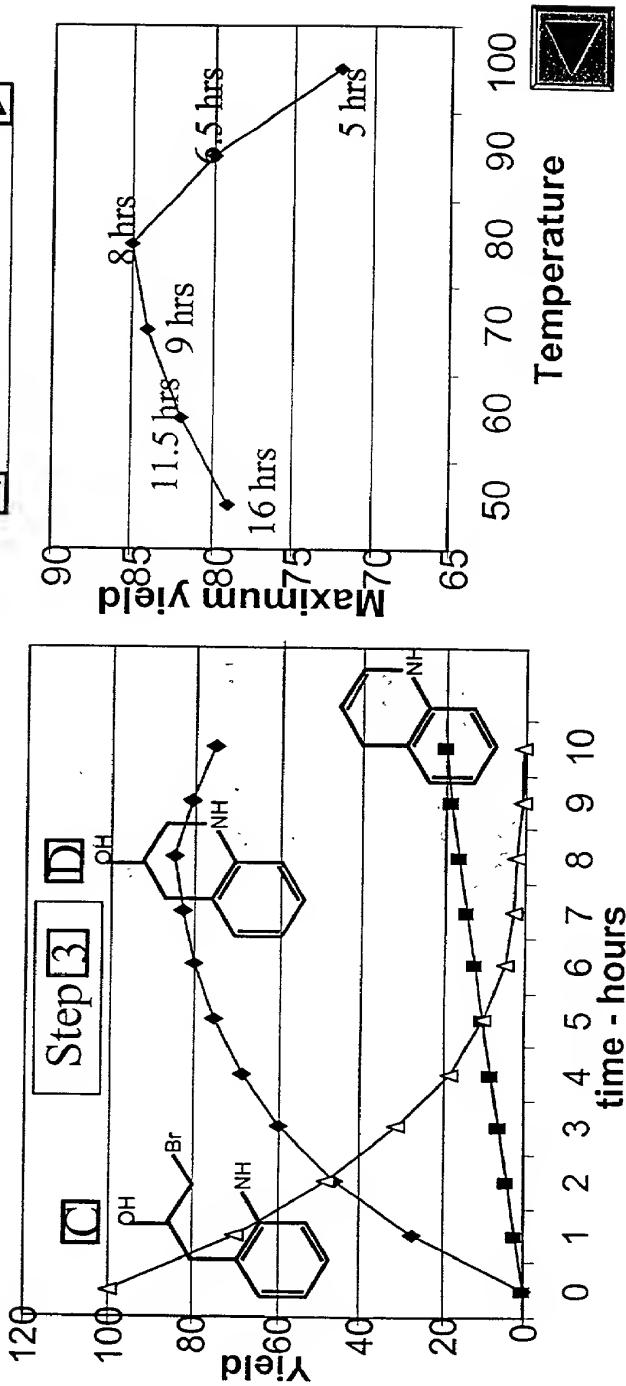
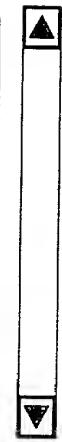
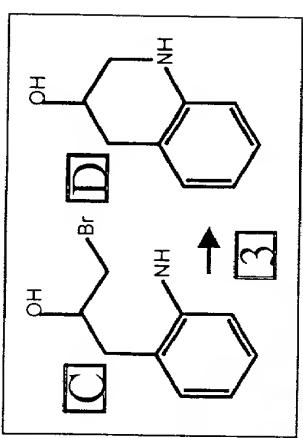
Step	Starting materials in order of addition	Amount (g)	Inventory ID and Location	Solvent	Amount (ml)	Recommended purification steps	Time	Temp.	Scheduled date for completion
3									

460

Fig. 10

Synthesis Reaction Optimization

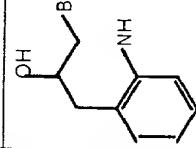
Optimize the Reaction Time and Temperature for Step [3]	
Temperature	80° C
Time	8 Hrs



480

Fig. 11

Request Bids

Target	Level of Confidentiality Required	Desired Quantity	Cost	Level of Purity	Stereochemical Requirements	Suggested Strategies	Request Bids	
							<input type="checkbox"/> Request Preliminary Bids	<input type="checkbox"/> Request Binding Bids
 <input type="checkbox"/> <input checked="" type="checkbox"/> <input type="checkbox"/>	Ultra High Medium Low None	10 g	< \$40,000	<input checked="" type="checkbox"/> 99% <input checked="" type="checkbox"/> 95% <input type="checkbox"/> 90%	None	<input type="checkbox"/> Edit		

500

Fig. 12